Communication Efficient Gaussian Elimination with Partial Pivoting using a Shape Morphing Data Layout

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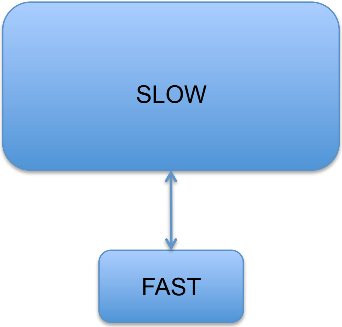
Summary

I'll present an algorithm for performing Gaussian elimination (i.e., computing an LU decomposition to solve a dense linear system) that

- is **communication optimal** and **cache oblivious**
  - matches the communication lower bounds for the sequential two-level memory model
  - requires no tuning to cache size
- is **numerically stable**
  - uses partial pivoting (row interchanges)
- uses a matrix data layout that changes on the fly
  - we call it **shape-morphing**

Two-Level Memory Model

- Computation happens only in fast memory (of size M)
- Matrix is too large to fit in fast memory
- Communication happens between slow and fast memory
- Words stored contiguously in slow memory can be read or written as a single message



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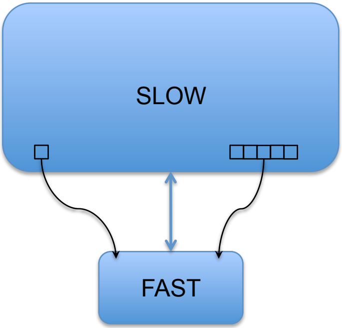

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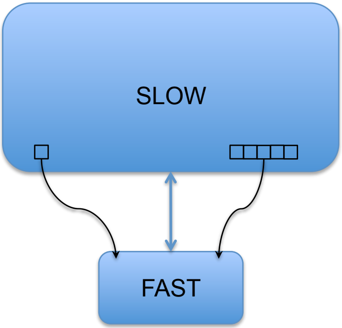

$$\text{runtime} = (\#\ \text{messages}) \cdot \alpha + (\#\ \text{words}) \cdot \beta + (\#\ \text{flops}) \cdot \gamma$$

We Have Four Metrics

For best performance on two-level memory model, we want to

(1) minimize words moved
(2) minimize messages moved

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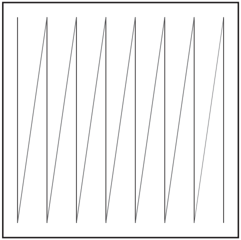
To get the right answer, we need to maintain

(4) numerical stability

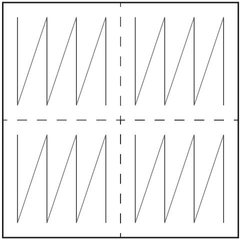
Summary Table

Algorithm	**Minimizes Words**	**Minimizes Messages**	**Cache Oblivious**	**Numerically Stable**
LAPACK [ABB+92]	✗	✗	✗	✓
Square-Recursive LU [BFJ+96]	✓	✓	✓	✗
Comm-Avoiding LU [GDX11]	✓	✓	✗	✓
Rectangular-Rec LU [Tol97]	✓	✗	✓	✓
Shape-Morphing LU	✓	✓	✓	✓

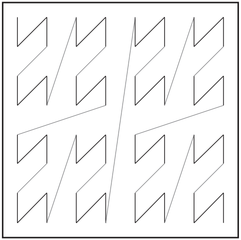
Recall: Matrix Data Layouts



Column Major



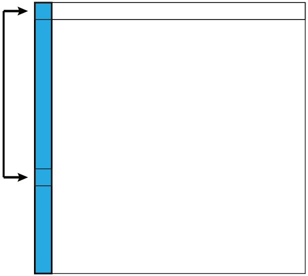
Block Contiguous



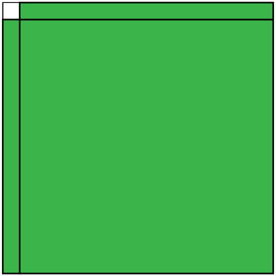
Block Recursive

- column major is most commonly used
- block contiguous has a block size parameter
- block recursive is also known as Morton ordering or bit-interleaved

Recall: (Naive) Gaussian Elimination with Partial Pivoting



Find pivot and scale column

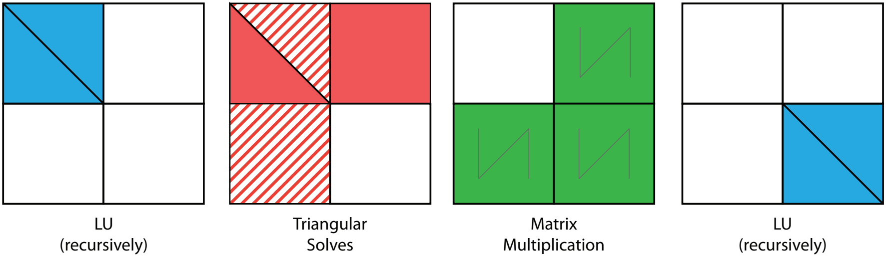


Update Schur complement

for each column:

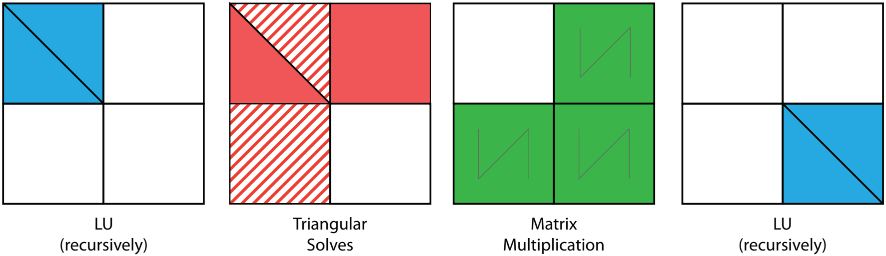
- pivot the largest entry to the diagonal
- divide the column by the diagonal entry
- perform rank-one update on the trailing matrix (Schur complement)

Square-Recursive Algorithm [BFJ+96]



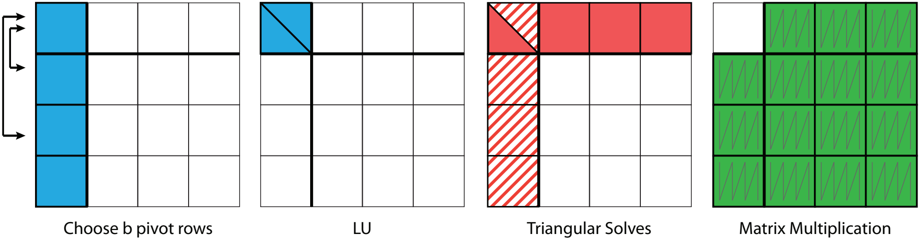
- maps to block recursive layout
- minimizes words and messages and is cache oblivious

Square-Recursive Algorithm [BFJ+96]



- maps to block recursive layout
- minimizes words and messages and is cache oblivious
- we forgot to pivot!
    - not numerically stable

Communication-Avoiding LU (CALU) Algorithm [GDX11]



- blocked algorithm, maps to block contiguous layout
- minimizes words and messages, but block size is cache aware
- pivoting scheme is different from partial pivoting, but almost as stable
    - called "tournament pivoting"

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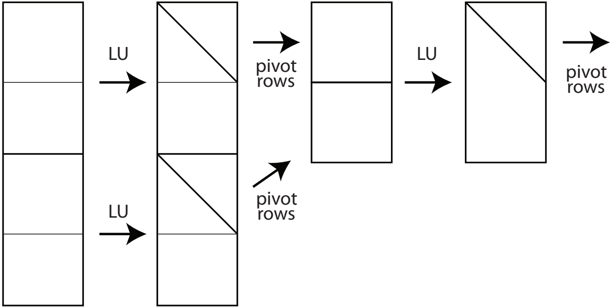

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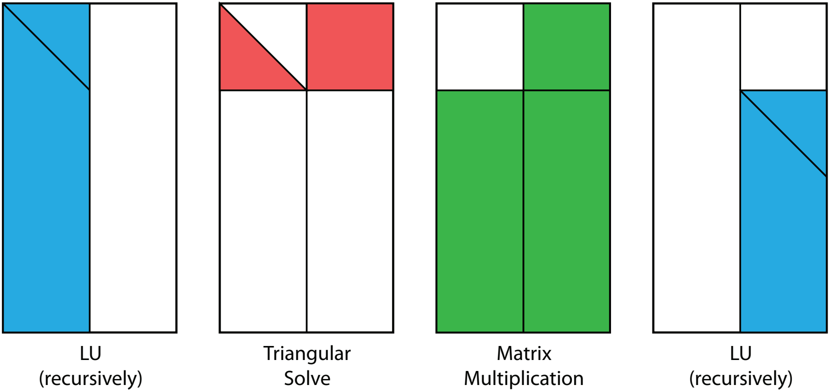
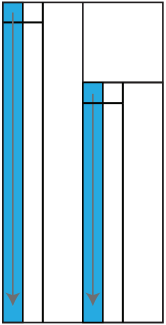
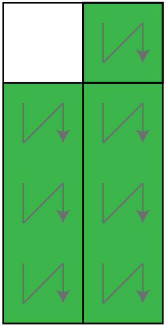
Rectangular-Recursive LU Algorithm [Tol97]



- minimizes words and is cache oblivious
- uses partial pivoting and so is numerically stable
- what data layout to use?

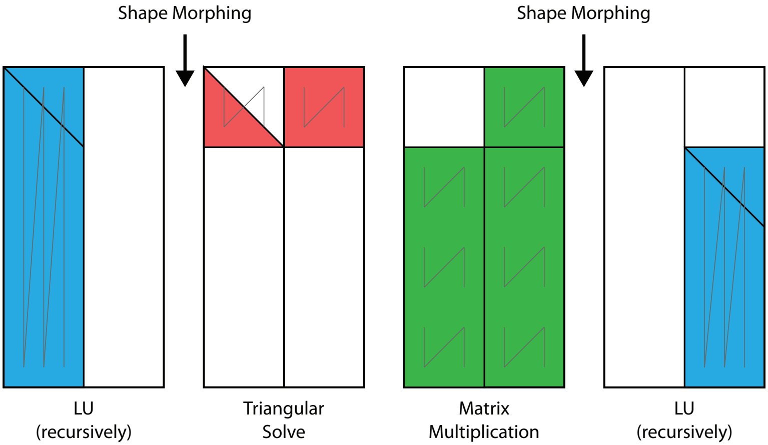
Data Layout Problem





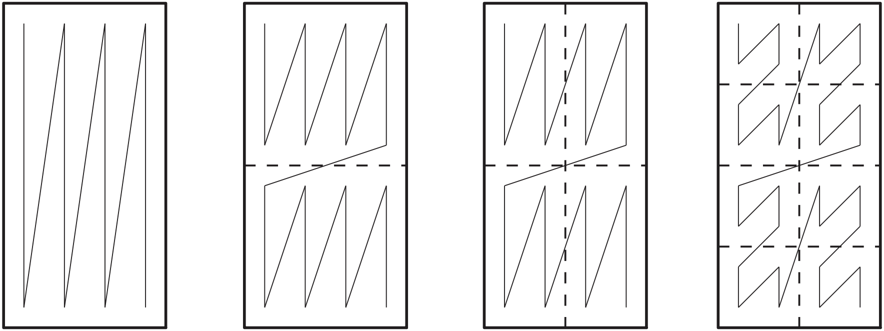
- Base case: find max element in column, pivot, and scale column
  - need column-major layout
  - recursive layout costs too many messages
- Subroutines: rectangular matrix multiplication and triangular solve
  - need recursive layout
  - column-major costs too many messages

Shape-Morphing LU Algorithm



- start and end in column-major layout
- switch to recursive for subroutine calls, then switch back

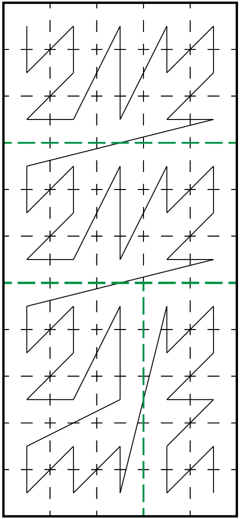
Main Idea: Shape Morphing



- convert between column-major and recursive layouts
- can be cache oblivious and communication efficient
- sacrifice some extra words moved (lower order term) in order to minimize messages

Other Complications

- rectangular recursive layout
  - generalizes Morton ordering
  - "split largest dimension"
- rectangular triangular solve
  - recursive algorithm
- applying pivots (row interchanges)
  - needs to be cache oblivious



Asymptotics

Algorithm	Words	Messages
Lower Bound [BDHS11, GDX11]	$\Omega\left(\frac{n^3}{\sqrt{M}}\right)$	$\Omega\left(\frac{n^3}{M^{3/2}}\right)$
CALU [GDX11]	$O\left(\frac{n^3}{\sqrt{M}} + n^2\right)$	$O\left(\frac{n^3}{M^{3/2}} + \frac{n^2}{M}\right)$
Rect-Rec LU [Tol97]	$O\left(\frac{n^3}{\sqrt{M}} + n^2 \log \frac{n^2}{M}\right)$	$O\left(\frac{n^3}{M} + \frac{n^2}{M} \log \frac{n^2}{M}\right)$
Shape-Morphing LU	$O\left(\frac{n^3}{\sqrt{M}} + n^2 \log^2 \frac{n^2}{M}\right)$	$O\left(\frac{n^3}{M^{3/2}} + \frac{n^2}{M} \log^2 \frac{n^2}{M}\right)$

n is matrix dimension, M is fast memory size

(this table assumes a square matrix, maximum message size of M)

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Discussion / Open Problems

- Same story for QR decomposition
  - shape morphing technique can be applied to a similar rectangular recursive algorithm with equivalent results
- Extension to parallel case is an open problem
  - tournament pivoting seems necessary in parallel case
  - data redistribution on the fly seems too expensive
- Performance data still needed
  - shape morphing will be most useful when latency costs are high and message sizes can be large (e.g., out-of-core computations)

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